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LOW ENERGY ELASTIC SCATTERING OF ELECTRON ON THE NEGATIVE IONS

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Abstract. In the framework of the many body theory we presented the method and results of calculations of the electron scattering on the negative ions. As an example we calculated the differential and total cross sections of the low energy elastic scattering of electrons on the negative ion Li^-.

1. INTRODUCTION

There have been a great interest for investigating photo absorption processes by negative ion lately (Buckman and Clark 1994, Ivanov 2004). This is connected with a great role of many electrons correlations and also with the appearance of lot of new characteristics related to the same processes with neutral atom. Electron scattering processes are less studied than processes of photodetachment. Scattering processes are interesting above all because of different polarization effects.

Regardless to Coulomb repulsion between the incident electron and ion, ion polarization influence special phase and cross section behaviour.

In this paper we have investigated elastic scattering electron on negative ions. The elastic electron scattering on Li^- is calculated here as an example. We used many-body theory method. The polarization effect is calculated t by solving Dyson equation (Amusia and Chernisheva 1997) and using improved random phase approximation which is developed in our early papers (Tančić et al. 1989). Because Li^- ion has closed shell and spherical symmetry the calculation is very simplified. In the paper, we used atomic system units.

2. THEORY

In the framework of the one particle model, the ground state wave functions are calculated in Hartree-Fock (HF) approximation. In this way we have taken into account only a part of many-electron correlations. In this calculation the HF approximation is initial approximation for developing different many-electron calculation. Total cross section for elastic scattering of electron with energy E and momentum $k = \sqrt{E}$ is

(Mott and Massey 1965)

$$\sigma(E) = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \left|1 - \exp(2i\delta_\ell(k))\right|^2, \tag{1}$$

where $\delta_\ell(k)$ is scattering phase of ℓ partial wave. The phase is determined by asymptotic form of scattered particle wave function (Drukarev G.F.: 1978)

$$\Psi_k(\vec{r}) = \frac{i}{2kr} \sum_i (2\ell+1) P_\ell(\cos\theta) \left[(-1)^\ell \exp(-ikr) - \exp(2i\delta_\ell(k) + ikr)\right] \tag{2}$$

There are two ways to calculate the scattering phase: 1. by solving HF equations for incident electron in the negative ion frozen core field, 2. by solving the integral equation which takes into account the core potential. The scattering phase is defined by the standard expression:

$$\delta_\ell = \arcsin\left(-\sqrt{\pi/k} \int_0^\infty J_\ell(kr) V(r) P_{N+1}(r) dr\right). \tag{3}$$

$J_\ell(kr)$ is the Bessel function, $V(r)$ scattering potential and $P_j(r)$ $j \in [1, S]$ (S is the number of the subshell in the ground ion state) is the radial function.

The polarization of core by incident electron is neglect in the HF approximation. The negative ion has a big polarisability because the external electrons are weakly bounded. The dynamic polarisability has calculated by Dyson equation method. The Dyson equation for the reducible self energy part $\tilde{\Sigma}$ of the one particle Green function has the form (Tančić and Nikolić 2002)

$$\left\langle E_1\ell|\tilde{\Sigma}(E)|E_2\ell\right\rangle = \langle E_1\ell|\Sigma(E)|E_2\ell\rangle + vp \int \langle E_2\ell|\Sigma(E)|E'\ell\rangle \left\langle E'\ell|\tilde{\Sigma}(E)|E_2\ell\right\rangle \frac{dE'}{E-E'}, \tag{4}$$

where $|E\ell\rangle$ are one electron wave functions. The $\langle\, |\Sigma(E)|\, \rangle$ is the irreducible self energy part of the Green function and may be derived in the form (Amusia et al. 1976):

$$\Sigma(E) = \Sigma^{HF}(E) + \Sigma^{cor}(E). \tag{5}$$

The matrix element $\Sigma^{cor}(E)$ in the lowest order on the perturbation theory (PT) of the Coulomb interaction is described by the diagrams of the second order (the first order of the PT is taken into account in the HF approximation). We have taken into account some important third order diagrams, too (improved version of the RPA method). The correction to the HF phase is defined by the expression:

$$\Delta\delta_\ell(E) = \arctan\left(-\pi \left\langle E\ell|\tilde{E}(E)\ell\right\rangle\right) \tag{6}$$

In the calculation of the phase correction (6) we used modified computer program (Amusia and Chernisheva 1997, Amusia et al. 1976). First the wave function for NI lithium ion ground state in HF approximation is calculated. Wave function and scattering phases of incident electron are determined in frozen field HF lithium negative ion. This function is used for the calculation of the matrix elements $\Sigma^{cor}(E)$ with $\Delta\ell = 0, 1, 2$. The scattering phases are determined by solving integral equation (4).

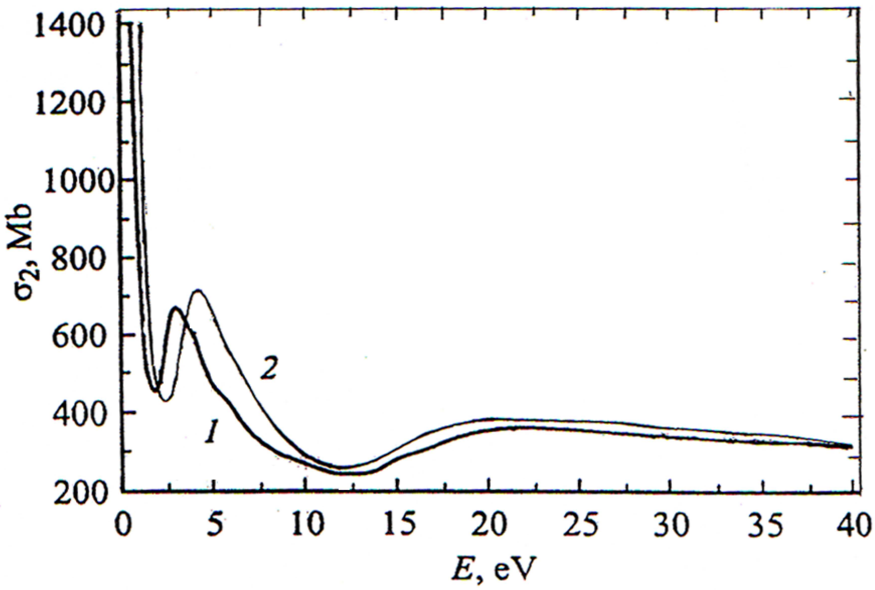

Figure 1: The total cross section of the electron elastic scattering on the litium negative ion. 1- Semennikhina V. Ivanov V.K., Lapkin C.V. 2004, 2- our improved calculations.

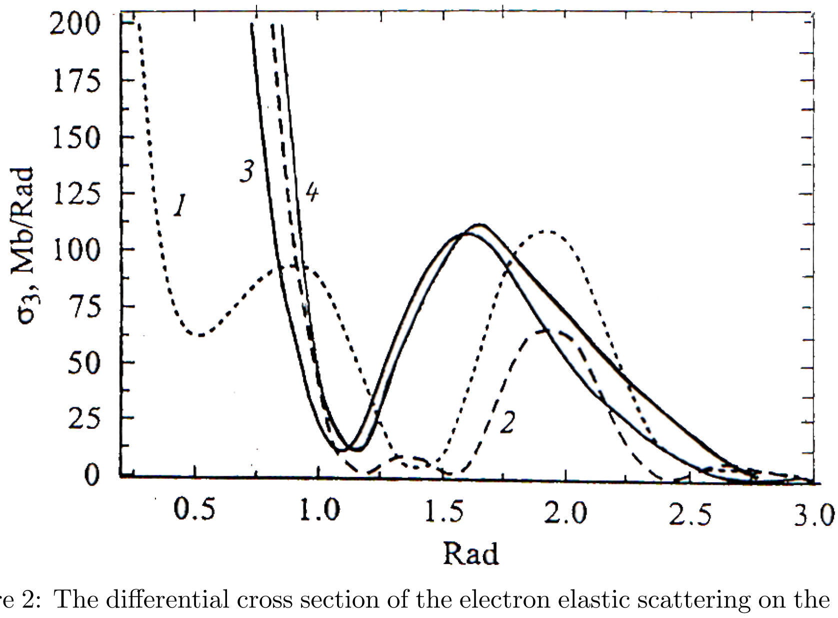

Figure 2: The differential cross section of the electron elastic scattering on the lithium negative ion at the electron energies: E=5 eV (1), E=15.5 eV (2), E=36 eV (3) Semennikhina et al. 2004. Our result (4) correspond to E=36 eV.

3. RESULTS AND CONCLUSIONS

Comparing the calculations of partial wave scattering phase on the repulsion Coulomb potential (CP) with HF calculations we can see: -Partial wave scattering phase on the CP is a smooth curve as function of incident electron energy. However, HF calculations of p and d partial waves show rough character of scattering phase. Leap appeared in p and d phase in order $\pi/4$ and $\pi/6$ respectively. This behaviour results from electron waves diffractions on space structure of negative ion.

The accounts achieved by Dyson equation method show that polarization potential changes essentially the behaviour of partial scattering phase: the leap in p-phase is now increased to $\pi/2$ order, while for d-phase that leaps is $\pi/3$ order when energy is $\approx 13.6eV$, and it practically cames only from many electron correlations. The influence of polarization potential decreases quickly with increasing of ℓ.

The behaviour of d phase is especially important because of many electron effects with energy $\approx 2.8eV$, interference minimum appears (when $\delta_d = \pi$, Fig. 1.).

As a conclusion we may notice that very interesting effects of electron scattering on negative ion are got and proved. The appearance of diffraction in electron scattering on negative ion leads to important changes in the scattering processes characteristics. The results show that it is very important to take into account the many body electron correlations. This account my be used on the other negative ions and negative charge clusters.

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